PRISMS-PF Application Formulation: dendriticSolidification

This example application implements a simple model of dendritic solidification based on the CHiMaD Benchmark Problem 3, itself based on the model given in the following article:
"Multiscale Finite-Difference-Diffusion-Monte-Carlo Method for Simulating Dendritic Solidification" by M. Plapp and A. Karma, *Journal of Computational Physics*, 165, 592-619 (2000)

1 Governing Equations

Consider a free energy density given by:

$$\Pi = \int_\Omega \left[\frac{1}{2} W^2(\hat{n}) |\nabla \phi|^2 + f(\phi, u) \right] \, dV \tag{1}$$

where ϕ is an order parameter for the solid phase and u is the dimensionaless temperature:

$$u = \frac{T - T_m}{L/c_p} \tag{2}$$

for temperature T, melting temperature T_m, latent heat L, and specific heat c_p. The free energy density, $f(\phi, u)$ is given by a double-well potential:

$$f(\phi, u) = -\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4 + \lambda u \phi \left(1 - \frac{2}{3}\phi^2 + \frac{1}{5}\phi^4 \right) \tag{3}$$

where λ is a dimensionless coupling constant. The gradient energy coefficient, W, is given by

$$W = W_0[1 + \epsilon_m cos[m(\theta - \theta_0)]] \tag{4}$$

where, W_0, ϵ_m, and θ_0 are constants and θ is the in-plane azimuthal angle, where $\tan(\theta) = fracn_y n_x$, where n_y and n_x are components of the normal vector $\hat{n} = \frac{\nabla \phi}{|\nabla \phi|}$.

The evolution equations are:

$$\frac{\partial u}{\partial t} = -\frac{\delta \Pi}{\delta \phi} = D \nabla^2 u + \frac{1}{2} \tau(\hat{n}) \frac{\partial \phi}{\partial t} \tag{5}$$

$$\tau(\hat{n}) \frac{\partial \phi}{\partial t} = [\phi - \lambda(1 - \phi^2)](1 - \phi^2) + \nabla \cdot [W(\hat{n})^2 \nabla \phi] + \frac{\partial}{\partial x} \left[|\nabla \phi|^2 W(\hat{n}) \frac{\partial W(\hat{n})}{\partial \left(\frac{\partial \phi}{\partial x} \right)} \right] \tag{6}$$

where

$$\tau(\hat{n}) = \tau_0[1 + \epsilon_m cos[m(\theta - \theta_0)]] \tag{7}$$

$$D = \frac{0.6267 \lambda W_0^2}{\tau_0} \tag{8}$$

2 Model Constants

W_0

τ_0

D

T_0

$\Delta = \frac{T_m - T_0}{L/c_p}$

3 Time Discretization

Considering forward Euler explicit time stepping, we have the time discretized kinetics equation:

$$\eta^{n+1} = \eta^n - \Delta t M_\eta \ ((f^n_{\beta,c} - f^n_{\alpha,c}) H^n_{,\eta} - \kappa \Delta \eta^n) \tag{9}$$

$$c^{n+1} = c^n + \Delta t M_\eta \ \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}(f^n_{\alpha,c}(1 - H^n) + f^n_{\beta,c} H^n)) \tag{10}$$

4 Weak Formulation

In the weak formulation, considering an arbitrary variation w, the above equations can be expressed as residual equations:

$$\int_\Omega w\eta^{n+1} \ dV = \int_\Omega w\eta^n - w\Delta t M_\eta \ ((f^n_{\beta,c} - f^n_{\alpha,c}) H^n_{,\eta} - \kappa \Delta \eta^n) \ dV \tag{11}$$

$$= \int_\Omega w \left(\underbrace{\eta^n - \Delta t M_\eta \ ((f^n_{\beta,c} - f^n_{\alpha,c}) H^n_{,\eta})}_{r_\eta} \right) + \boldsymbol{\nabla} w \cdot \underbrace{(-\Delta t M_\eta \kappa) \boldsymbol{\nabla} \eta^n}_{r_{\eta x}} \ dV \tag{12}$$

and

$$\int_\Omega w c^{n+1} \ dV = \int_\Omega w c^n + w \Delta t M_c \ \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}(f^n_{\alpha,c}(1 - H^n) + f^n_{\beta,c} H^n)) \ dV \tag{13}$$

$$= \int_\Omega w \underbrace{c^n}_{r_c} + \boldsymbol{\nabla} w \underbrace{(-\Delta t M_c) \ [\ (f^n_{\alpha,cc}(1 - H^n) + f^n_{\beta,cc} H^n) \boldsymbol{\nabla} c + \ ((f^n_{\beta,c} - f^n_{\alpha,c}) H^n_{,\eta} \boldsymbol{\nabla} \eta)]}_{r_{cx}} \ dV \tag{14}$$

The above values of r_η, $r_{\eta x}$, r_c and r_{cx} are used to define the residuals in the following parameters file: *applications/coupledCahnHilliardAllenCahn/parameters.h*